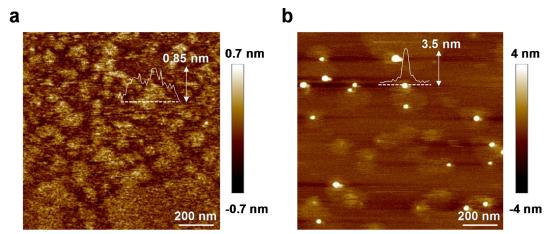
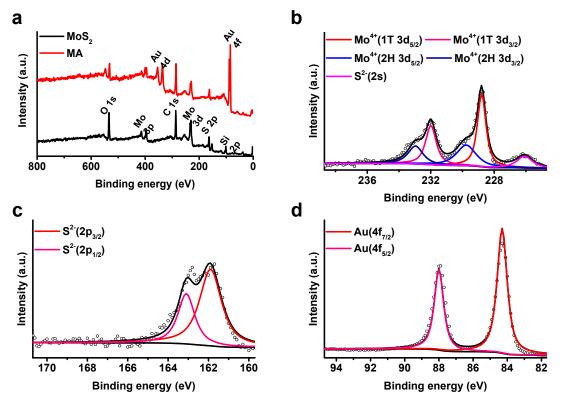
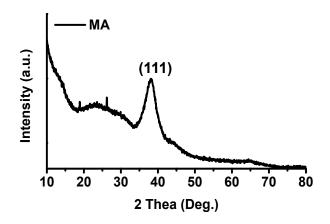
## **Supplementary Information**



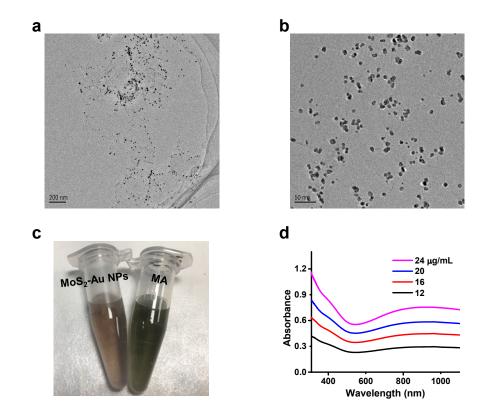
**Supporting Figure S1.** AFM images and the corresponding line profiles of (a)  $MoS_2$  nanosheets and (b) MA nanostructures.



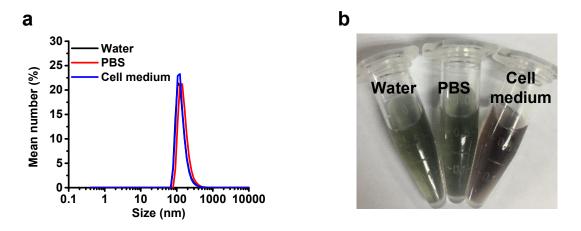
**Supporting Figure S2.** XPS characterization of  $MoS_2$  before and after the in-situ growth of Au nanoislands. (a) XPS spectra of  $MoS_2$  nanosheets and MA nanostructures on SiO<sub>2</sub> substrates. (b) Mo scans. (c) S scans. (d) Au scans.



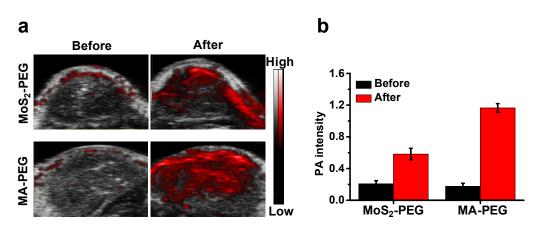
Supporting Figure S3. XRD spectrum of MA nanostructures.



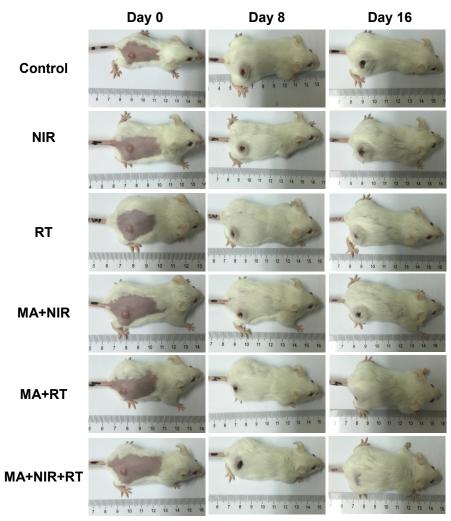
**Supporting Figure S4.** Comparison of two kinds of  $MoS_2$ -Au nanocomposites. (a) TEM image of  $MoS_2$ -Au NPs showing that the Au NPs were grown on the surface of  $MoS_2$  nanosheets. (b) Enlarged TEM image showing that all of the Au nanomaterials grew on the  $MoS_2$  nanosheets were nanoparticles with lateral size of several nanometers. (c) Photos of  $MoS_2$ -Au NPs and MA solutions. (d) Absorbance spectra of MA with various concentrations.



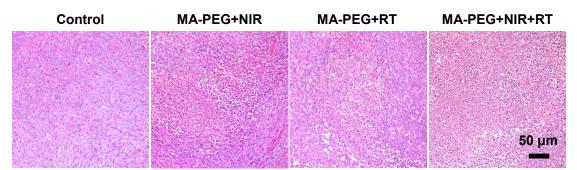
**Supporting Figure S5.** Physiological stability tests of MA-PEG. (a) The hydrodynamic size of MA-PEG in various solutions measured by dynamic light scattering. (b) The photo of various MA-PEG solutions (from left to right: water, PBS, cell culture medium) after one-week incubation, showing no aggregation or precipitation.



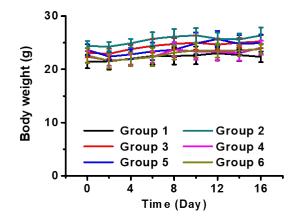
**Supporting Figure S6.** Comparison of PA imaging ability of  $MoS_2$ -PEG and MA-PEG. (a) PA images of tumor before and after the injection of  $MoS_2$ -PEG and MA-PEG. (b) The corresponding PA intensity values of tumors presented in (a).



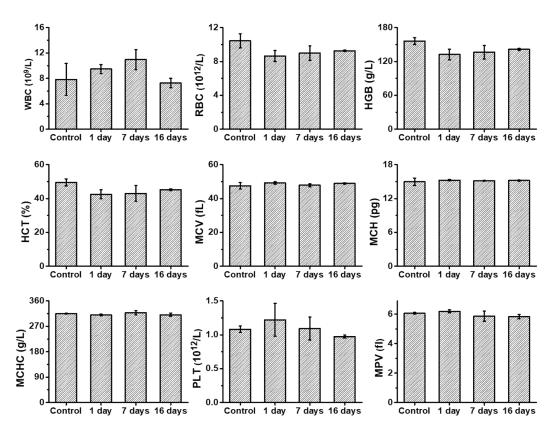
Supporting Figure S7. Photos of mice with various treatment at different time points.



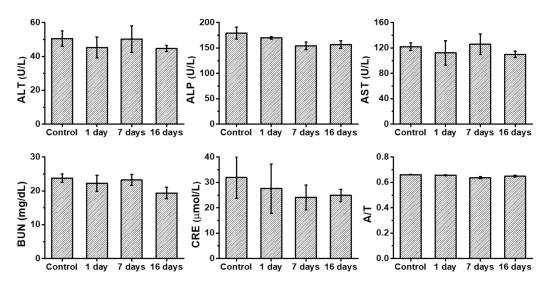
Supporting Figure S8. H&E stained tumor slices from the mice 1 day after each treatment.



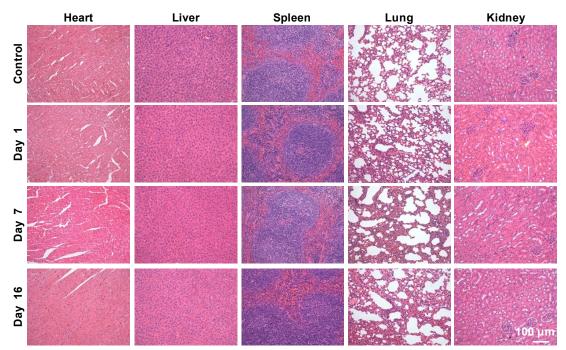
**Supporting Figure S9.** Body weight change curves of mice during 16 days after various treatments (Group 1: Control, Group 2: NIR only, Group 3: RT only, Group 4: MA-PEG+NIR, Group 5: MA-PEG+RT, Group 6: MA-PEG+NIR+RT).



**Supporting Figure S10.** Hematology data of mice sacrificed at 1 day, 7 days and 16 days after injection of MA-PEG nanostructures, including white blood cells (WBC), red blood cells (RBC), hemoglobin (HGB), hematocrit (HCT), mean corpuscular volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin concentration (MCHC), platelets (PLT), and mean platelet volume (MPV).



**Supporting Figure S11.** Serum biochemistry data of mice sacrificed at 1 day, 7 days, and 16 days after injection of MA-PEG nanostructures, including alanine aminotransferase (ALT), alkaline phosphatase (ALP), aspartate aminotransferase (AST), blood urea nitrogen (BUN), creatinine (CRE), and albumin/globin ratio (A/T).



**Supporting Figure S12.** H&E stained tissue slices of major organs (heart, liver, spleen, lung, and kidney) in sacrificed mice 1 day, 7 days, and 16 days after injection of MA-PEG nanostructures.